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Progress Report

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Studies of Elementary Reactions of Chemical Importance in the Atmospheres of Planets

Fred L. Nesbitt, Principal Investigator

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Reactions investigated and completed during the period of this progress report included N + C_2H_3 --> prod (1), O + HOBr --> prod (2) and F + C_2H_5OH --> Prod (3). Reactions (2) and product radicals from reaction (3) are important in models of the Earth's stratosphere, while reaction (1) is pertinent to our understanding of the chemistry of Titan and Neptune.

Reaction (1) was investigated at 298 K and 1 Torr total pressure. The absolute rate constant and branching ratios were measured. The rate constant was determined under pseudo-first-order conditions with $[N]_0 > [C_2H_3]_0$. The result is $k_1 = (8.9\pm2.8)\times10^{-11}$ cm^3 $molecule^{-1}$ s^{-1}. Three primary channels were observed: N + C_2H_3 --> C_2H_2 + NH (1a), CH_2CN + H (1b) and CH_3CN (1c). The following branching ratios were measured at T=298 K: $\Gamma_{1a} = 0.16$, $\Gamma_{1c} = 0.04$. Since no other products were detected, we infer that channel (1b) accounts for most if not all of the remaining products, i.e. $\Gamma_{1b} = 0.80$.

Reaction (2) was investigated as a function of temperature at 1 torr total pressure. The reaction was investigated under pseudo-first-order conditions with $[O]_0 > [HOBr]_0$.
The temperature range is 233 K to 423 K and derived Arrhenius expression is $(1.4\pm0.5)\times10^{-10}\exp[(-430\pm260)/T]$ cm^3 $molecule^{-1}$ s^{-1}.

Reaction (3) was investigated at 223 to 423K and one Torr total pressure. A discharge flow reactor with mass spectrometric detection was used to determine the fractional yield of ethoxy from the reaction of F and C_2H_5OH. The purpose of this study was to establish reaction (3) as a convenient source ethoxy radical and to report the yield over the temperature range 223 to 423K. The

fractional yield experiments were preformed at GSFC while the threshold and photoionization spectrum were measured at Brookhaven National Laboratory. The fractional yield was 0.62±0.08 at 298K. The threshold and photoionization experiments are still being analyzed.